Notes on the Numerical Solution of the Diffusion Equation with the Finite Difference Method

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Contents

1 Introduction 1
2 One-dimensional unsteady diffusion equation 2
3 Basic Finite Different schemes 3
  3.1 Explicit FTCS Method 3
  3.2 Implicit BTCS Method 4
4 The Crank-Nicolson Method 4

1 Introduction

The numerical treatment of partial differential equations is, by itself, a vast subject. Partial differential equations are at the heart of many if not most, computer analyses or simulations of continuous physical systems, such as fluids, electromagnetic fields, the human body, and so on.

Several general techniques for solving PDEs have been investigated for over a century. Roughly speaking, we can mention, for instance:

1. Separation of Variables (SoV) method.

2. Integral-equation methods.

3. Analytical methods based on integral transforms like Fourier or Laplace transforms, and finally.

4. Numerical methods.

Often it is very difficult or impossible to obtain analytical solutions; in this case, the only option is to implement numerical techniques. Numerical methods permit us to solve very complicated problems; however, much of the physics involved in the analytical solutions is often lost.

This document presents the standard numerical solution of the one-dimensional unsteady diffusion equation based on the Finite Difference method. It has been written as a primary support material for the undergraduate course of Electrodynamics. Our main goal is to apply this theory to solve numerically the paraxial scalar wave equation to propagate one-dimensional wave profiles.

2 One-dimensional unsteady diffusion equation

We begin by writing the one-dimensional unsteady diffusion equation

$$\kappa \frac{\partial^2 f}{\partial x^2} = \frac{\partial f}{\partial t} \tag{1}$$

where κ is the *diffusion coefficient* and it is assumed to be positive, and $f = f(x,t)$ may represent any diffusive physical quantity, for example the temperature, the optical paraxial scalar field, or the wave function in the time-dependent Schrödinger equation..

The solution is to be found subject to the initial condition $f(x,0) = F(x)$, where $F(x)$ is a known function. The domain of the solution extends over the range $a \leq x \leq b$.

The one-dimensional unsteady diffusion equation is a parabolic differential equation in time with a well-known analytical solution given by

$$f(x,t) = \frac{1}{\sqrt{4\pi\kappa t}} \int_{-\infty}^{\infty} F(x+u) \exp\left(-\frac{u^2}{4\kappa t}\right) \,\mathrm{d}u, \tag{2}$$

for κ constant.

The solution to the problem is confined in a two-dimensional grid that covers the strip $a \leq x \leq b$ and $0 \leq t \leq t_{\max}$ in the space-time space plane, see Fig. 1.

Our objective is to compute the values of the function f_i^n, at the grid points x_i, $i \in [1, ..., K+1]$, at a sequence of successive time levels t^n, beginning from the initial time level $t^0 = 0$, and subject to the boundary conditions $f(a,t) = f_1^n = 0$ and $f(b,t) = f_{K+1}^n = 0$.

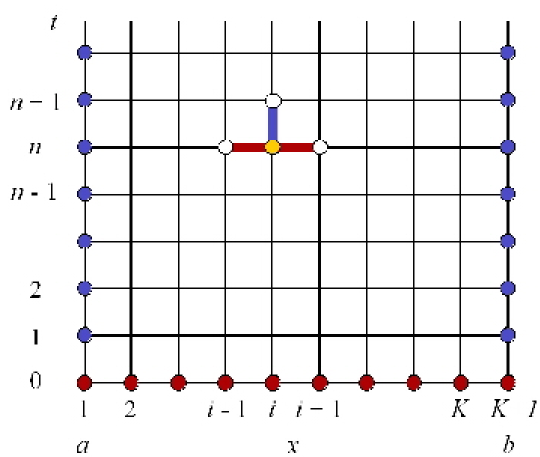

Figure 1: Computational grid showing the (x,t) space-time plane for the one-dimensional diffusion equation and the FTCS method.

3 Basic Finite Different schemes

3.1 Explicit FTCS Method

We now approximate the time derivative in Eq. (1) with a first-order forward difference, and the space derivative with a second-order centered difference

$$\kappa\left[\frac{f_{i+1}^{n}-2f_{i}^{n}+f_{i-1}^{n}}{\Delta x^{2}}\right]=\frac{f_{i}^{n+1}-f_{i}^{n}}{\tau},$$

where τ is the time increment. FTCS means Forward Time Centered Space [1].

Solving above equation for f_i^{n+1}, we obtain

$$f_{i}^{n+1}=\alpha f_{i-1}^{n}+(1-2\alpha)\,f_{i}^{n}+\alpha f_{i+1}^{n}, \tag{3}$$

where

$$\alpha\equiv\frac{\kappa\tau}{\Delta x^{2}} \tag{4}$$

is a number called *diffusion number.* Equation (3) can be applied to internal grid points $i=2,...,K$ but not at the boundary points $i=1$ and $i=K+1$.

FTCS provide us with a straightforward algorithm to compute f at level $n+1$ in terms of the values of f at level n.

The method is called *explicit* since it does not require inverting a matrix or solving a system of algebraic equations.

The matrix representation of the method is as follows

$$\mathbf{f}^{n+1}=\mathbf{A}\mathbf{f}^{n}=\begin{bmatrix}1-2\alpha & \alpha & 0 & 0\\ \alpha & 1-2\alpha & \ddots & 0\\ 0 & \ddots & 1-2\alpha & \alpha\\ 0 & 0 & \alpha & 1-2\alpha\end{bmatrix}\mathbf{f}^{n}, \tag{5}$$

where the vectors involve only the interior grid points

$$\mathbf{f}^{n}=\begin{bmatrix}f_{2}^{n}\\ f_{3}^{n}\\ \vdots\\ f_{K}^{n}\end{bmatrix}, \tag{6}$$

and $\mathbf{A}$ is a $(K-1)\times(K-1)$ *propagating* square matrix.

In order to apply the method, we start with the initial condition $\mathbf{f}^0=\mathbf{F}(x)$, now we use the Eq. (5) to calculate the function f at time $t=1*\tau$, in other words $\mathbf{f}^1$. The procedure is repeated until the desired time is reached.

The stability of the numerical algorithm will depend on the properties of the propagating matrix $\mathbf{A}$. The von Neumann analysis is one of the most used test to check the stability of the Finite-Difference methods [1].

Performing the von Neumann analysis we can find that the FTCS algorithm is stable only when

$$\alpha<\frac{1}{2},$$

so the FTCS method is *conditionally stable.*

3.2 Implicit BTCS Method

We have considered first the explicit methods where the solution at a particular time level is computed directly from the solution at one or two previous levels, without solving any systems of equations. We turn now to considering implicit discretizations that require solving systems of equations.

Applying the diffusion equation Eq. (1) at point x_i at the instant t^{n+1}, and approximating the temporal derivative with a backward derivative and the spatial derivative with a central difference, we obtain the BTCS difference equation

$$\kappa\left[\frac{f_{i+1}^{n+1}-2f_i^{n+1}+f_{i-1}^{n+1}}{\Delta x^2}\right]=\frac{f_i^{n+1}-f_i^n}{\tau}.$$

Rearranging

$$-\alpha f_{i-1}^{n+1}+\left(1+2\alpha\right)f_i^{n+1}-\alpha f_{i+1}^{n+1}=f_i^n. \tag{7}$$

Recasting the above equation into a matrix form we obtain the linear system of equations $\mathbf{B}\mathbf{f}^{n+1}=\mathbf{f}^n$, which can be written explicitly as

$$\mathbf{f}^{n+1}=\mathbf{B}^{-1}\mathbf{f}^n=\begin{bmatrix}1+2\alpha & -\alpha & 0 & 0\\ -\alpha & 1+2\alpha & 0 & 0\\ 0 & 0 & 1+2\alpha & -\alpha\\ 0 & 0 & -\alpha & 1+2\alpha\end{bmatrix}^{-1}\mathbf{f}^n \tag{8}$$

In practice, in order to compute the solution at the $n+1$ time level, we solve the system of linear algebraic equations $\mathbf{B}\mathbf{f}^{n+1}=\mathbf{f}^n$.

By performing the von Neumann test we can corroborate that the BTCS is a unconditionally stable.

4 The Crank-Nicolson Method

Continuing our search for an efficient method, we target an algorithm that is second order accurate in both time and space and unconditionally stable. To this end, we recall that the explicit FTCS method emerged by applying the Diffusion Eq. (1) at point x_i at the time level t^n, whereas the implicit BTCS method emerged by applying the Diffusion equation at point x_i at the time level t^{n+1}.

We now apply Eq. (1) at the intermediate grid point $\left(x_i, t^{n+1/2}\right)$ that os located halfway between the grid points (x_i, t^n) and $\left(x_i, t^{n+1}\right)$, set the spatial derivative at the $t^{n+1/2}$ level equal to the average value of the spatial derivative derivatives at the t^n and t^{n+1} levels, and arrive at the finite-difference equation

$$\kappa\frac{1}{2}\left[\frac{f_{i+1}^{n+1}-2f_i^{n+1}+f_{i-1}^{n+1}}{\Delta x^2}+\frac{f_{i+1}^{n}-2f_i^{n}+f_{i-1}^{n}}{\Delta x^2}\right]=\frac{f_i^{n+1}-f_i^n}{\tau}. \tag{9}$$

The corresponding finite-difference scheme is shown in Fig. 2.

Rearranging above equation, we obtain a tridiagonal system of equations

$$-\alpha f_{i-1}^{n+1}+2\left(1+\alpha\right)f_i^{n+1}-\alpha f_{i+1}^{n+1}=\alpha f_{i-1}^n+2\left(1-\alpha\right)f_i^n+\alpha f_{i+1}^n. \tag{10}$$

This scheme is widely known as the **Crank-Nicolson Method**, and it is a second-order accurate in both time and space. Recasting Eq. (10) into a matrix form, we obtain the system of linear equations

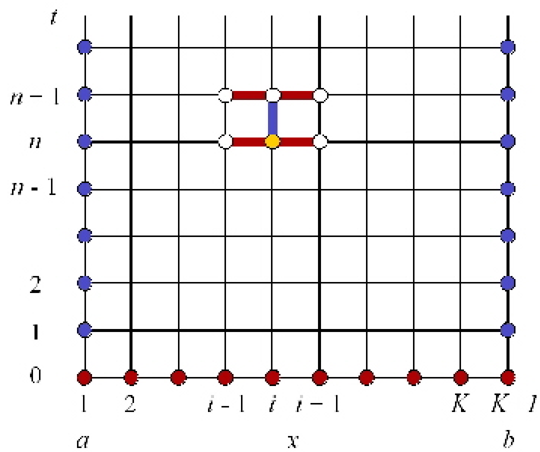

Figure 2: Computational grid showing the (x, t) space-time plane for the one-dimensional diffusion equation using Crank-Nicolson scheme.

$\mathbf{C}\mathbf{f}^{n+1} = \mathbf{D}\mathbf{f}^{n}$, namely

$$\begin{bmatrix} 2\,(1+\alpha) & -\alpha & 0 & 0 \\ -\alpha & 2\,(1+\alpha) & \ddots & 0 \\ 0 & \ddots & 2\,(1+\alpha) & -\alpha \\ 0 & 0 & -\alpha & 2\,(1+\alpha) \end{bmatrix} \mathbf{f}^{n+1} = \begin{bmatrix} 2\,(1-\alpha) & \alpha & 0 & 0 \\ \alpha & 2\,(1-\alpha) & \ddots & 0 \\ 0 & \ddots & 2\,(1-\alpha) & \alpha \\ 0 & 0 & \alpha & 2\,(1-\alpha) \end{bmatrix} \mathbf{f}^{n}.$$

Solving for $\mathbf{f}^{n+1}$ yields

$$\boxed{\mathbf{f}^{n+1} = \left[\mathbf{C}^{-1}\mathbf{D}\right] \mathbf{f}^{n} = \mathbf{P}\ \mathbf{f}^{n}} \tag{11}$$

which shows that stepping in time is equivalent to mapping with the propagating matrix $\mathbf{P} \equiv \mathbf{C}^{-1}\mathbf{D}$.

Carrying out the von Neumann stability analysis confirm us that the Crank-Nicolson method is unconditionally stable [1].

Because of its qualities with respect to both accuracy and stability, the Crank-Nicolson method has become a standard choice in practice.

References

[1] Richard L. Burden, J. Douglas Faires, *Numerical Analysis,* (Brooks/Cole Pub Co., 2001)

[2] C. Pozrikidis, *Numerical Computation in Science asnd Enginnering,* (Oxford University Press, 1998)